

# Photon and Neutron Open Science Cloud - PaNOSC

**Workshop on EOSC – Implementation steps**

**3 December 2019**

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**Venue: Technology Centre of the CAS**



# PaNOSC factsheet

Call: **Horizon 2020 InfraEOSC-04**

Partners: **ESRF, ILL, XFEL.EU, ESS, CERIC-ERIC, ELI-DG, EGI**

Description: **cluster of ESFRI Photon and Neutron sources**

Observers/non-funded: **GÉANT, EUDAT, national RIs**

Linked 3<sup>rd</sup> parties via EGI: **DESY, STFC, CESNET**

Status: **Started 1/12/2018**

Github: <https://github.com/panosc-eu>

Home page: <https://panosc.eu>

Twitter: [@PaNOSC\\_eu](#) [#PaNOSC](#)

Budget: **12 M€**

Coordinator: **ESRF**

Started: **1/12/2018**

Duration: **4 years**



# ELI in Brief

- ELI ERIC will be the world's most advanced **laser research infrastructure**
- First **international research infrastructure** built completely in **Central Europe**
- Funded in synergy between **ESIF, National and Framework** funds, after **EU approval** and delivered through a community effort



An aerial photograph of the ELI-ALPS facility. The main building is a large, modern structure with a blue roof and a glass facade. It is surrounded by green lawns and parking areas. In the background, there is a large, rectangular building with a brown roof and the 'ei' logo on its side. The overall scene is a well-maintained industrial or research complex.

# ELI-ALPS

*X-UV and X-ray fs/atto-pulses, for  
temporal investigation of dynamics in  
atoms, molecules, plasmas and solids.*

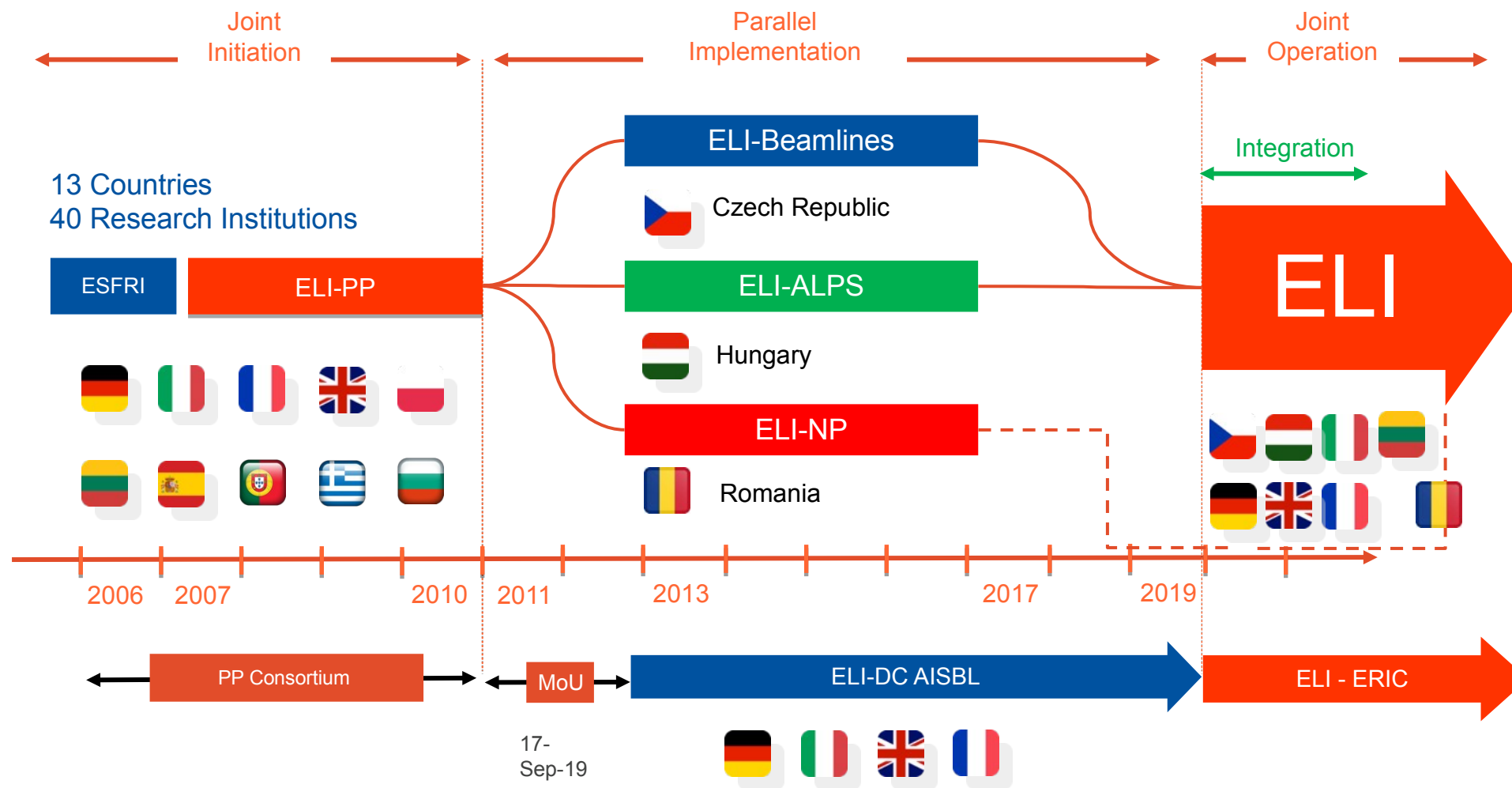
# ELI BEAMLINES

An aerial architectural rendering of the ELI Beamlines facility. The main building is a large, rectangular structure with a flat roof and a grid-like pattern of skylights. It is surrounded by parking lots filled with cars, landscaped green areas with trees and walkways, and other smaller buildings in the background. The scene is set in a suburban or semi-rural area with more buildings and trees visible in the distance.

*The forefront of high-intensity, high-energy  
density, short-pulse laser systems*

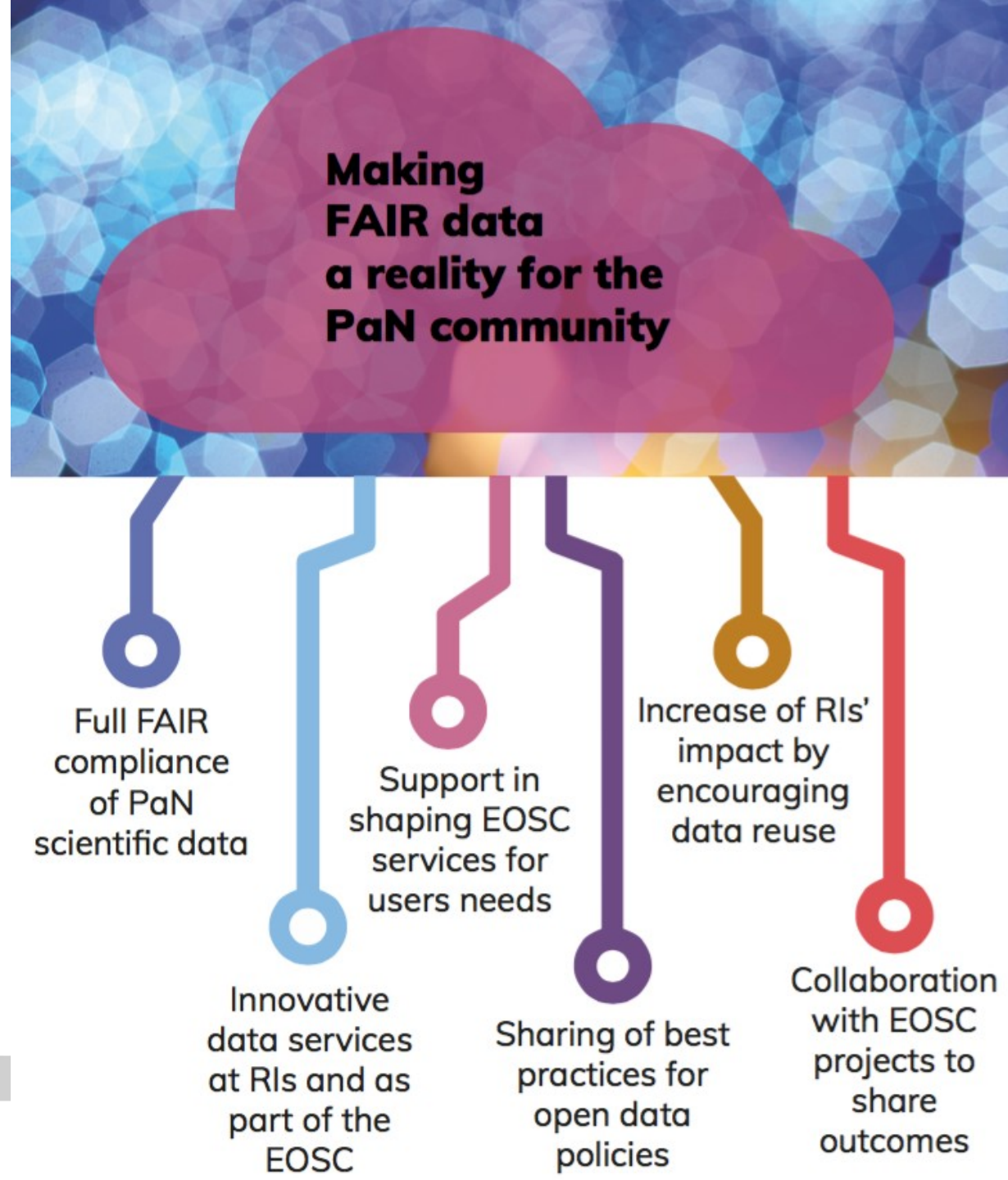


# ELI Timeline



# PaNOSC goals

PaNOSC works closely with the PaN sources in Europe to develop common policies, strategies and solutions in the area of FAIR data policy, data management and data services, integrating them into the EOSC.



# Data policy WP

WP2

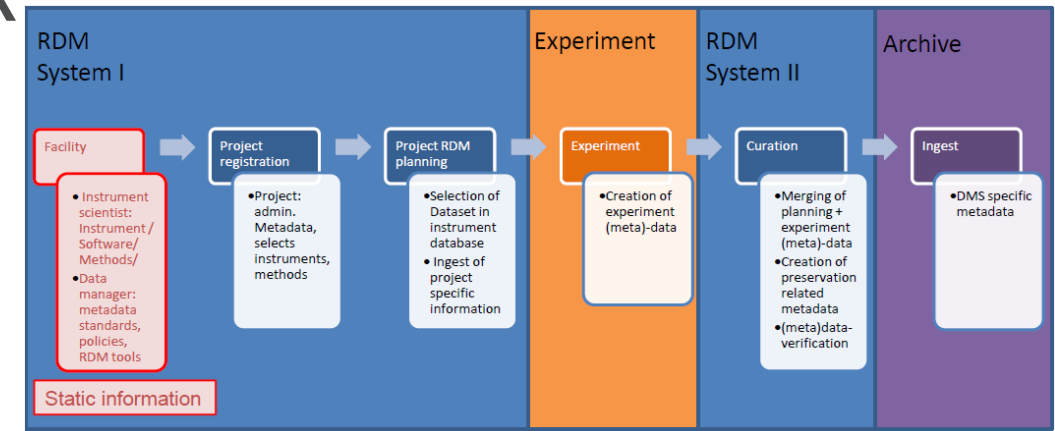
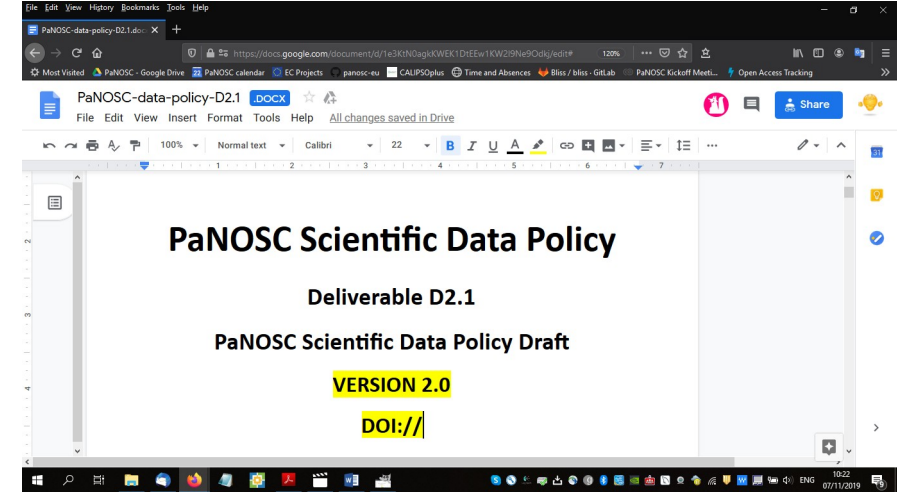
Update the PaNdata data policy

Include the FAIR concepts and make it FAIR compliant

Update existing Data Policies to be compatible with the Data Policy 2.0 framework

Develop a tool for Data Management Plans together with ExPaNDS

Share outcomes with ExPaNDS





# Data catalogue WP

Develop an Application Programmers Interface (API) for searching for FAIR data

Integrate search API into EOSC portal

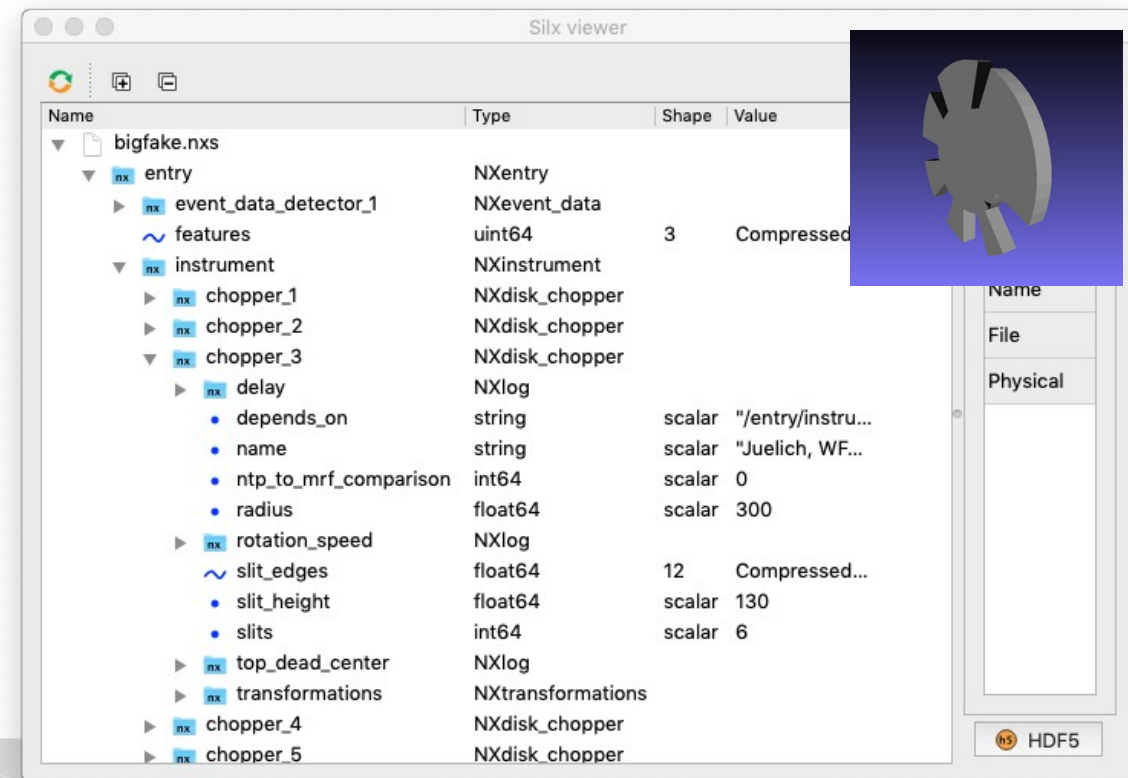
Use Nexus/HDF5 for metadata as much as possible

Enhance, extend and improve NeXus

Collect of metadata on beamlines

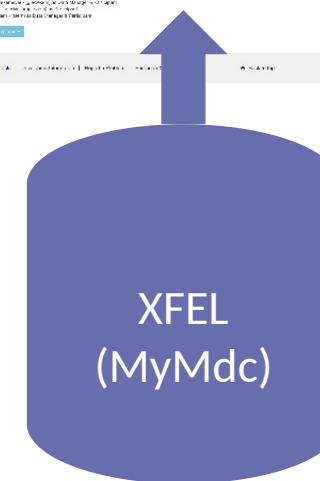
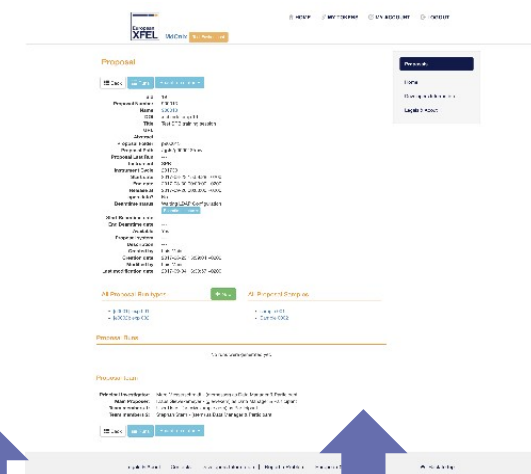
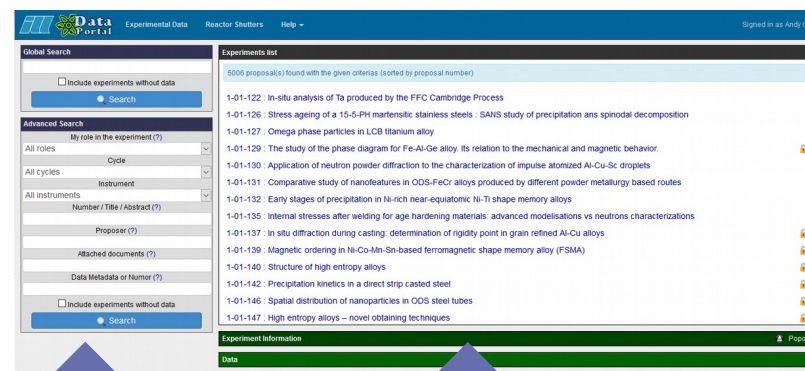
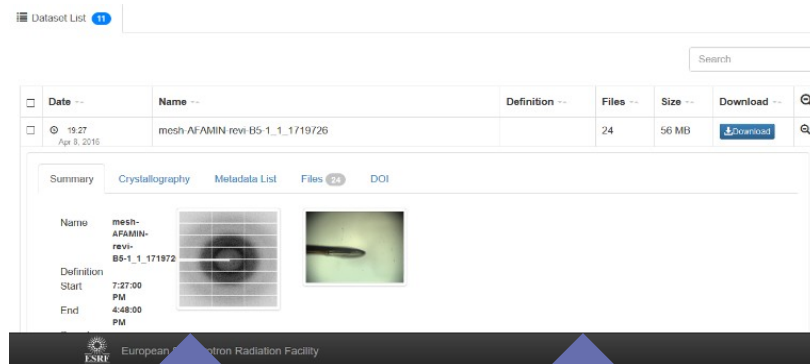
Share outcomes with ExPaNDS

Dataset			Show/Hide	List Operations	Expand Operations
PATCH	/Datasets	Patch an existing model instance or insert a new one into the data source.			
GET	/Datasets	Find all instances of the model matched by filter from the data source.			
PUT	/Datasets	Replace an existing model instance or insert a new one into the data source.			
POST	/Datasets	Create a new instance of the model and persist it into the data source.			
PATCH	/Datasets/{id}	Patch attributes for a model instance and persist it into the data source.			
GET	/Datasets/{id}	Find a model instance by {{id}} from the data source.			
HEAD	/Datasets/{id}	Check whether a model instance exists in the data source.			
PUT	/Datasets/{id}	Replace attributes for a model instance and persist it into the data source.			
DELETE	/Datasets/{id}	Delete a model instance by {{id}} from the data source.			
GET	/Datasets/{id}/exists	Check whether a model instance exists in the data source.			



# PaNOSC has 6 data catalogues with different APIs + UIs

WP3



# PaNOSC common API across all sites



Search for Datasets



Common API to search across all PaNOSC catalogues

ESRF  
(icat)

CERIC  
(icat)

ESS  
(SciCat)

ILL  
(local)

ELI  
(tbd)

XFEL  
(MyMdc)

# Data Analysis Services WP

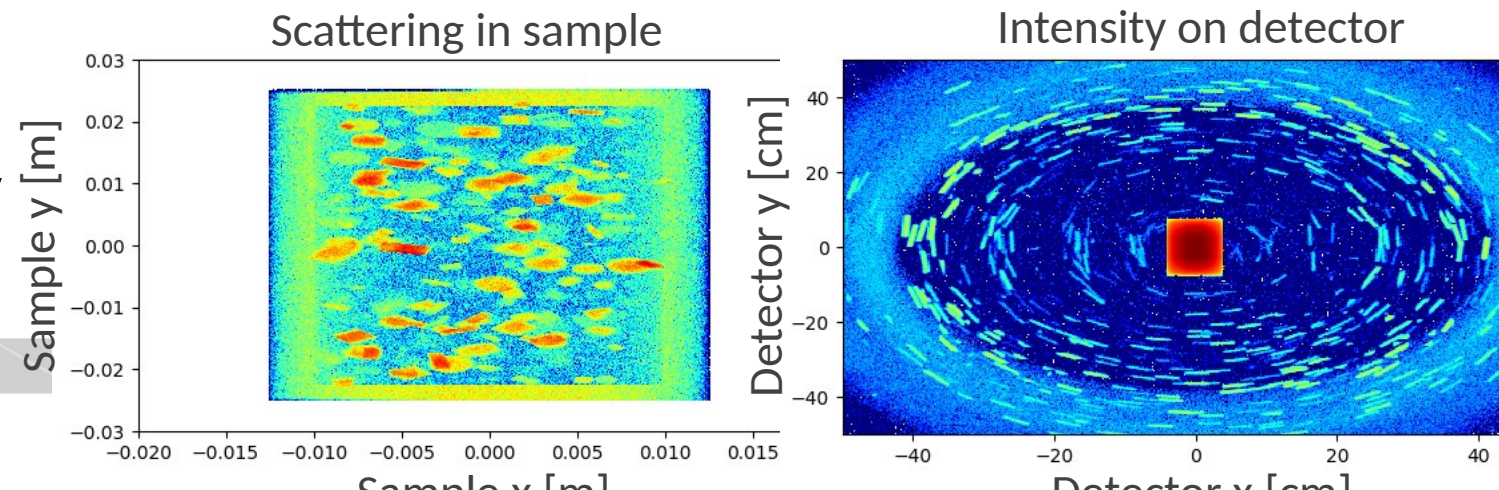
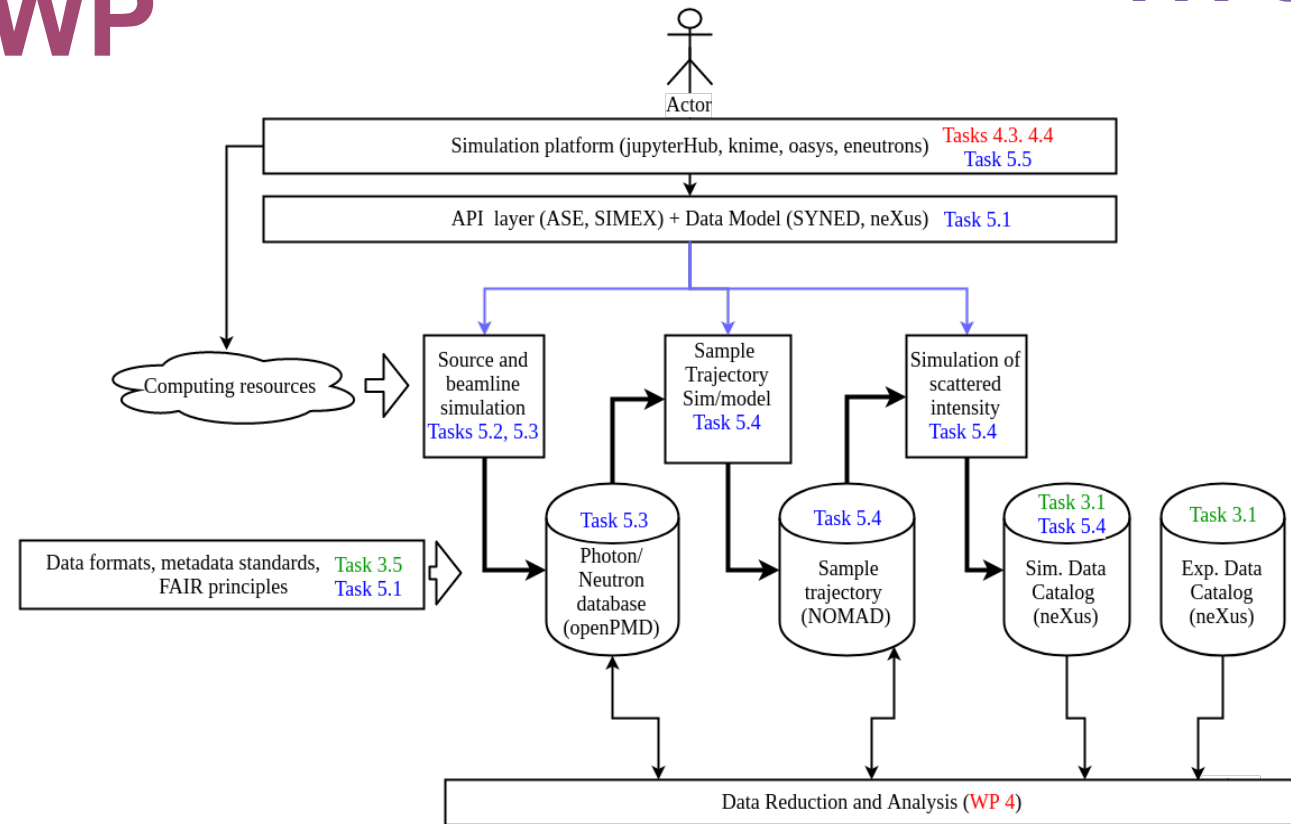
- Jupyter Notebooks
- Remote Desktop in Browser
- Remote data analysis portal
- HDF5 and visualisation in notebooks
- Package software for s/w catalogue





# Simulation services WP

- **SIMEX**: Start-to-end photon experiment simulation library (python)
- **McStas-script**: python API for Neutron ray-tracing with McStas
- **OASYS**: Wavefront propagation for beamline design (WISE)
- **EPOCH** particle in cell + McStas: Simulation of laser driven neutron sources and ray tracing





# EOSC Integration WP

- **AAI = Authentication and Authorisation Infrastructure**
  - Critical if we want to identify people and define roles
  - EOSC must solve at least the AAI problem
  - PaNOSC is working with Geant to make UmbrellaId sustainable
- **Develop a PaNOSC data analysis as a service portal**
- **Integrate PaNOSC services into EOSC**
- **Data download service + Software catalog service**

- **3 uses cases :**

1. User driven data transfer (e.g. **Globus Online**)
2. Data archiving for RI (**STFC as the archive center**)
3. Transfer from RI to compute facilities on behalf of users (i.e. based on the scenario where users perform analysis on a different infra than the one of the RI where the data have been produced). Currently exploring **OneData**, **dCache** and simple solution without caching (**webdav**)

# Sustainability WP

- **Develop a model to calculate cost of FAIR data**
- **Propose a sustainability plan for Ris**
- **Develop models for different service levels**
- **Participate and contribute to EOSC Sustainability**



# Training + e-learning WP

e-neutrons.org

Wiki with neutron scattering theory  
Web instrument simulation using McStas  
Quizzes using both theory and simulation

Migration to ESS servers underway

Extensions:

- Support for Jupyter Notebooks
- Integrate data analysis services
- Integrate simulation services

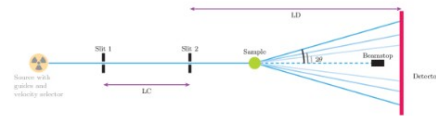
**McStas** sim.e-neutrons.org WP8

Apple Remote ...e (kickstart) SpinW Software for ...el Computers Studierende sa... | Dikatal.dk Bachmann N S...4896 | eBay Bachmann Tr...t C...

Instrument

Logged in as mcstas (see recent simruns) Logout

SANSsimple (click for documentation)



Parameters for SANSsimple

pinhole\_rad [m]: 0.004 radius of the collimating pinholes (0.004)  
LC [m]: 3 length of the collimator - distance between pinholes (3)

MediaWiki

Page Discussion

## Inelastic nuclear neutron scattering

One of the early successes of neutron scattering was the study of dynamics of matter, in particular phonon dispersion relations. Here, the vibrational frequency (or phonon energy) is deduced from the change in neutron energy through the principle of energy conservation. Hence, for the study of dynamics we are dealing with inelastic neutron scattering.

This page naturally leads to the description on the [Scattering from lattice vibrations](#) page of neutron scattering from quantised lattice vibrations, or *phonons*. The related topic of inelastic neutron scattering from diffusion and molecular motion is not covered in this version of the notes.

Instrumentation for the general field of inelastic neutron scattering is described on the [Instrumentation](#) page.

**Contents [hide]**

- 1 \*Scattering theory for nuclear dynamics
- 1.1 \*Scattering from initial to final state
- 1.2 \*The observable nuclear cross section

### \*Scattering theory for nuclear dynamics

We will now return to the basic scattering theory from the [Basics of neutron scattering](#) page to derive the equations that govern all inelastic scattering from nuclei.

### \*Scattering from initial to final state

In the [master scattering equation](#) on the [Basics of neutron scattering](#) page, we derived the starting equation for the inelastic cross section:

$$(1) \quad \frac{d^2\sigma}{d\Omega dE_f} \Big|_{\lambda_i \rightarrow \lambda_f} = \frac{k_f}{k_i} \left( \frac{m_n}{2\pi\hbar^2} \right)^2 \left| \langle \lambda_f | \hat{V} | \lambda_i \rangle \right|^2 \delta(E_f - E_i + \hbar\omega).$$

We begin by expanding the expression for the nuclear potential on the [Small angle neutron scattering](#) page:

$$(2) \quad \hat{V} = \frac{2\pi\hbar^2}{m_n} \sum_j b_j \delta(\mathbf{r} - \mathbf{R}_j),$$

where  $\mathbf{R}_j$  is now the operator for the position of the  $j$ 'th nucleus. We use this to expand the matrix element in the inelastic cross section:

$$(3) \quad \begin{aligned} \left| \langle \lambda_f | \hat{V} | \lambda_i \rangle \right|^2 &= \left( \frac{2\pi\hbar^2}{m_n} \right)^2 \left| \sum_j b_j \langle \lambda_f | \delta(\mathbf{r} - \mathbf{R}_j) | \lambda_i \rangle \right|^2 \\ &= \left( \frac{2\pi\hbar^2}{m_n} \right)^2 \sum_{j,j'} b_j b_{j'} \langle \lambda_f | \exp(-iq \cdot \mathbf{R}_j) | \lambda_i \rangle \langle \lambda_i | \exp(iq \cdot \mathbf{R}_{j'}) | \lambda_f \rangle. \end{aligned}$$

If all nuclei were fixed in position, we would now reach the diffraction cross section by summing over the (in practice unmeasurable) finite states of the lattice,  $|\lambda_i\rangle$ , since the  $\delta$ -function in (1) would factorize out and vanish by integration. However, we cannot do this simple calculation now, so we need to take a more difficult path. We rewrite the troublesome delta-function in (1), using  $2\pi\delta(x) = \int_{-\infty}^{\infty} \exp(iax) dx$  (following Squires<sup>[1] 2.3</sup>):

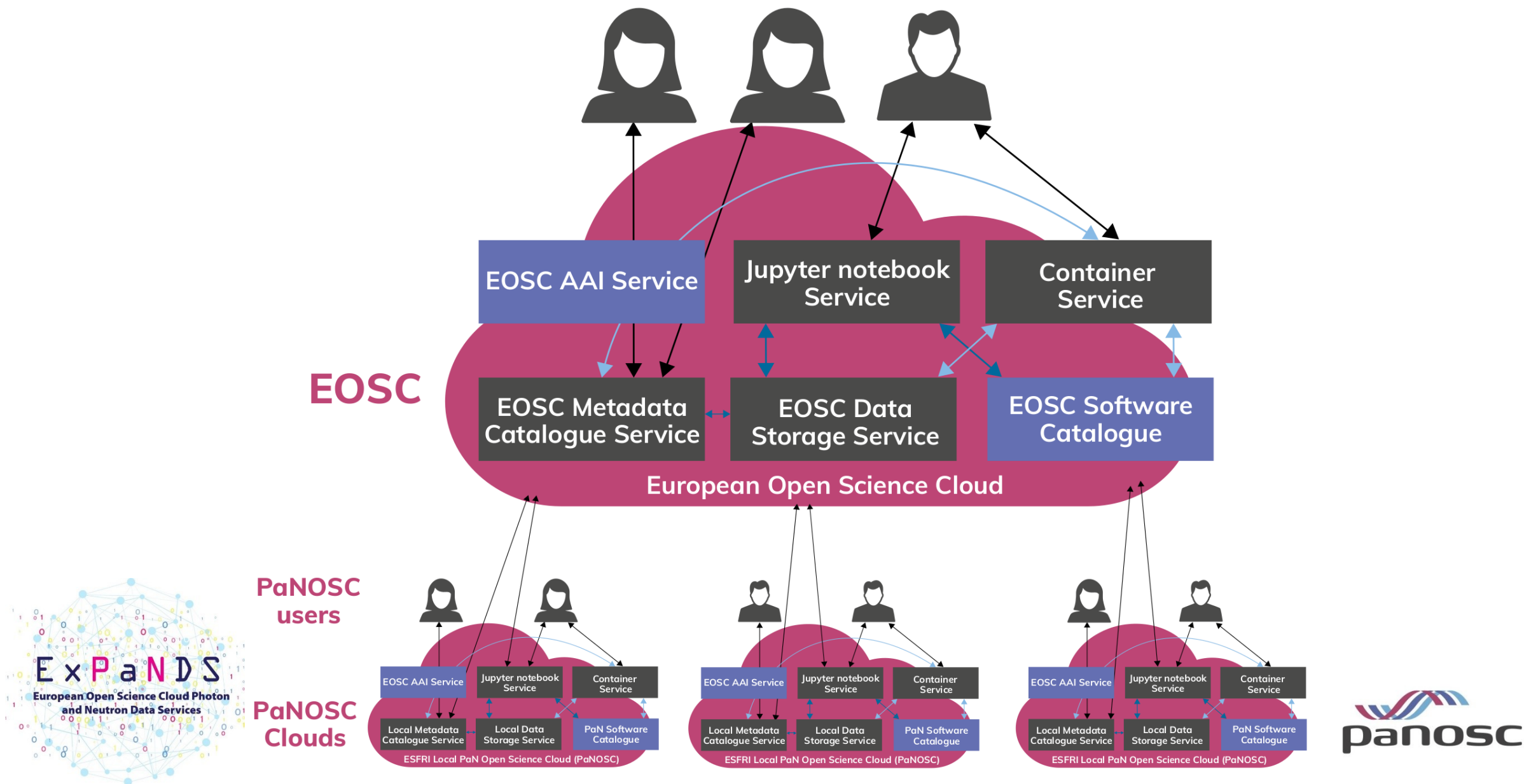
$$(4) \quad \delta(E_f - E_i + \hbar\omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \exp\left(\frac{i(E_f - E_i)t}{\hbar}\right) \exp(-i\omega t) dt.$$

Now, we utilize a rather intuitive identity from quantum mechanics, valid when  $|\lambda\rangle$  is an eigenstate of the Hamiltonian  $H$  with eigenvalue  $E_\lambda$ :

$$(5) \quad \exp\left(\frac{iHt}{\hbar}\right) |\lambda\rangle = \exp\left(\frac{iE_\lambda t}{\hbar}\right) |\lambda\rangle.$$


# Our Vision – a PaN scientific commons

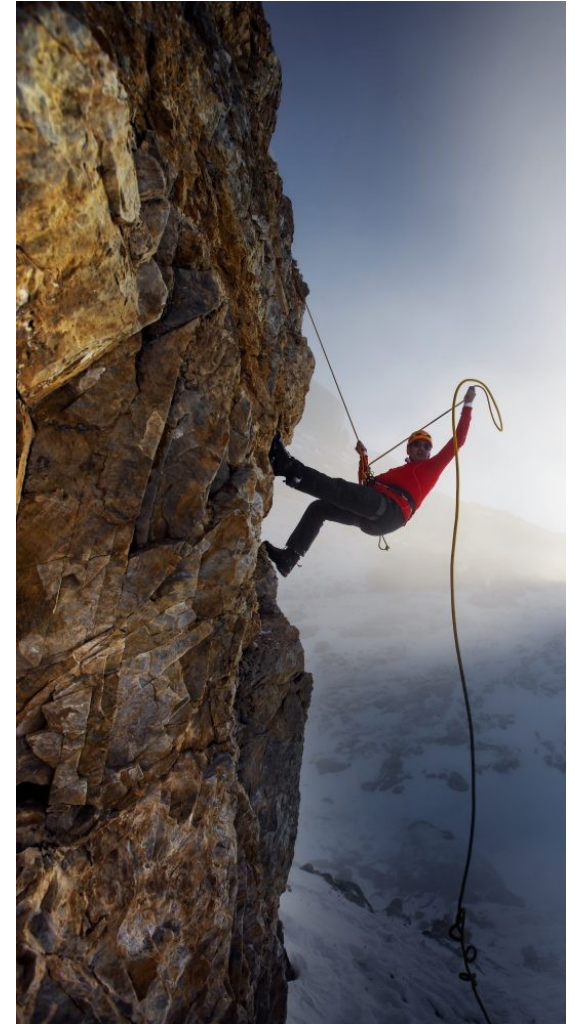
ALL





# ELI in PaNOSC

- The amount of data will not be the main challenge (10+ PB of archived data per annum)
- Standardisation challenge (approach to metadata, detectors, etc.) as priority
- Cultural issue within due to a “lab approach” to experimental data (no significant experience on making data available and (re-)usable within the community)
- PaNOSC is helping structuring the thought and policy process:
  - Consortium gives access to resources and experience
  - Commitment to adopting PaNOSC Data Policy Framework
  - Push for integration of data-related activities within ELI
  - Push for long-term vision in terms of services
  - Cross-community approach



# CESNET in PaNOSC

- Third-party partner, together with DESY, lead by EGI.eu
- WP6 – cloud provider, integrated in EGI FedCloud, in EOSC Marketplace
  - Support for data transfer use-cases
    - OneData use-case
  - Support for JupyterHub integration
    - Already running on CESNET, integrated into EGI/EOSC-hub infrastructure
- AAI lead by GEANT, federated solution based on EduTeams
  - CESNET provides one key component (Perun)

# Conclusion

1. **PaNOSC vision is to create a Scientific Data Commons for Photon and Neutron sources and make the data available via the EOSC**
2. **PaNOSC will collaborate closely with ExPaNDS to make FAIR data a reality for all PaN RIs**
3. **PaNOSC has been running for 1 year and is now up to speed**
4. **PaNOSC will allow us to address the data analysis problem**



# PaNOSC Resources

- <https://panosc.eu>
- <https://github.com/panosc-eu/panosc>
- “Enabling Open Science for Photon and Neutron sources”  
presented at ICALEPCS 2019  
<http://icalepcs2019.vrws.de/papers/tubpl02.pdf>
- Calipsoplus JRA2 – “Building a Data Analysis as a Service Portal”  
presented at ICALEPCS 2019  
<http://icalepcs2019.vrws.de/papers/wepha057.pdf>

